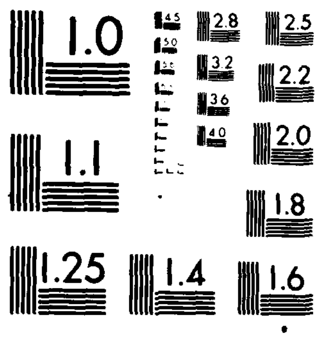
AD-A110 008 MICHIGAN STATE UNIV EAST LANSING DEPT OF CHEMISTRY F/6 9/2
COMPUTERS IN SCIENTIFIC INSTRUMENTATION.(U)
JAN 82 C G ENKE N00014-76-C-1092
UNCLASSIFIED TR-7 NL

END
DATE
FILMED
3-82
DTIC


1.0
4.5
5.0
2.8
2.5
3.2
2.2
3.6
4.0
2.0
1.1
1.8
1.25
1.4
1.6

LEVEL II

(13)

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Seven	2. GOVT ACCESSION NO. AD-A110008	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Computers in Scientific Instrumentation		5. TYPE OF REPORT & PERIOD COVERED Interim Technical Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Christie G. Enke		8. CONTRACT OR GRANT NUMBER(s) N00014-76-C-1092
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Chemistry Michigan State University East Lansing, MI 48824		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Chemistry Program Office of Naval Research Arlington, VA 22217		12. REPORT DATE January 13, 1982
		13. NUMBER OF PAGES
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) ONR Representative Ohio State University Research Center 1314 Kinnear Road Columbus, OH 43212		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release, distribution unlimited.

DTIC ELECTE JAN 25 1982 E

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

(12) 14

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The rapid evolution of computer applications in scientific instrumentation is briefly traced from early data processing to modern computer-based instruments. Computer and interface developments have both contributed to this evolution. The form of the computer used strongly affects the ease of instrument operation and the degree of functional adaptability. Probable pathways toward instruments with increased "intelligence" include the development and intelligent control of powerful "multidimensional" instruments, the implementation of

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-014-6601

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

01 25 82 096

hierarchical computer networks and multiprocessor controllers, and the simplification of programming. The importance of the scientist's involvement in these developments is discussed.

DISCLAIMER NOTICE

THIS DOCUMENT IS BEST QUALITY PRACTICABLE. THE COPY FURNISHED TO DTIC CONTAINED A SIGNIFICANT NUMBER OF PAGES WHICH DO NOT REPRODUCE LEGIBLY.

OFFICE OF NAVAL RESEARCH

Contract N00014-76-C-1092

Task No. NR 051-634

TECHNICAL REPORT NO. 7

Computers in Scientific Instrumentation

by

Christie G. Enke

Prepared for Publication

in

SCIENCE Magazine

Department of Chemistry
Michigan State University
East Lansing, MI 48824

January 13, 1982

To Appear in Science, Feb. 12, 1982

Article

Computers in Scientific Instrumentation

C. G. Enke

The author is a professor of chemistry at Michigan State University, East Lansing 48824.

Summary. The rapid evolution of computer applications in scientific instrumentation is briefly traced from early data processing to modern computer-based instruments. Computer and interface developments have both contributed to this evolution. The form of the computer used strongly affects the ease of instrument operation and the degree of functional adaptability. Probable pathways toward instruments with increased "intelligence" include the development and intelligent control of powerful "multidimensional" instruments, the implementation of hierarchical computer networks and multiprocessor controllers, and the simplification of programming. The importance of the scientist's involvement in these developments is discussed.

In the beginning (about 30 years ago), when all computers were large and very expensive, they existed only in the inner sancta of the computer centers of large institutions. Most programs and data were carried to the computer in the form of punched cards and the line printer output was retrieved hours or days later. Then, at some point in the steady decrease in the size and cost of computers, the minicomputer entered the scientific laboratory. It enabled the computer to collect data directly from the instruments and also perform some limited data processing. This was the beginning of computers in scientific instrumentation, and for many scientists the "laboratory computer" became a new and exciting tool (*1*). When the computer was dedicated to a single instrument, it was able to control the instrument and perform the data collection process. Early applications of dedicated computers were all with costly instruments such as x-ray diffractometers, but as computers continued to decrease in cost and size, so did the scale of instruments to which they could be dedicated. The last great leap in this evolution has been the incorporation of the remarkably inexpensive and tiny microprocessor to instruments of every type from spectrophotometers to balances and *p*H meters.

In this article, I will discuss some of the benefits of instrument computerization and some of the forms computerized instruments can take. Since instruments and other devices that incorporate computers are now sometimes called intelligent, it is fair to wonder what new functions "intelligent" instruments will provide. Possible improvements in both the convenience and the capability of instruments will be discussed, as well as the factors that now appear to limit the rate or extent of improvement. We are certainly not limited by computer technology itself; the hardware has much more capability than is exploited in current instrumentation. However, it is not clear which disciplines and institutions will provide the concepts and devices needed for the new breed of instruments.

Attachment, Absorption, and Transformation

For direct application in scientific instrumentation the computer must be able to acquire data from one or more sensors in the instrument and control some aspects of the instrument's operation. The circuits that provide these key links in the instrument-computer interaction are called interfaces. As shown in this section, the ease of interfacing determines the degree of involvement of the computer in the instrument functions and thus strongly affects the sophistication of the resulting computerized instrument. The concurrent evolution of both computing systems and interfacing techniques has been essential in achieving the present state of the art.

Interfacing. Computers have an internal data communication pathway called a bus, illustrated in Fig. 1, through which memory and all sources or destinations of data are connected to the central processing unit (CPU) (2). The CPU and bus in the computer are analogous to the brain and spinal cord in the body. All data on the bus are in digital form—signals in one of two states (high or low). Each such signal represents 1 bit (binary digit) of information. A combination of n bits, called a word can encode any integer from 0 to 2^n-1. Digital words can be transmitted by sending the bit signals sequentially in a single channel (serial form) or simultaneously in multiple channels (parallel form). The CPU bus uses parallel digital lines for data and address communication. Data are transmitted on the bus only at appropriate times as determined by control signals from the CPU.

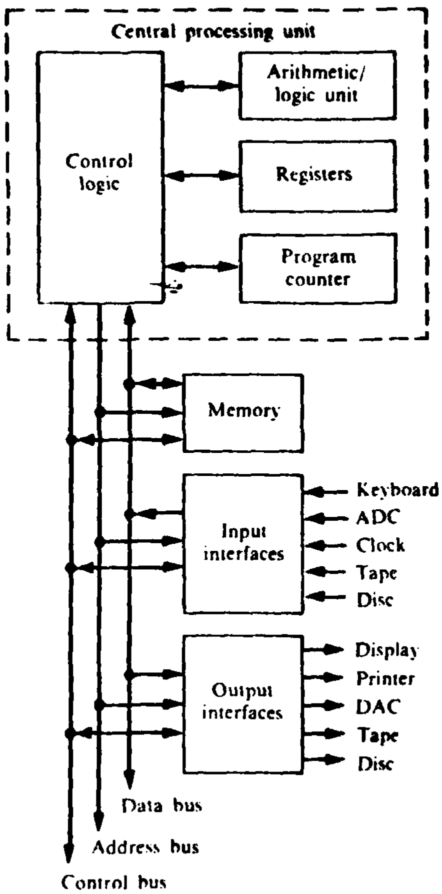


Fig. 1. Structure of a basic digital computer. The CPU acquires and executes the instructions. The program is stored in a section of memory reserved for that purpose. The CPU supervises communication along the shared data bus by using the address bus to specify the source or destination of the data. The program counter supplies the address of the instruction to be executed. The control bus contains data direction, timing, and special control signals. [From (2).]

A complete interface must accomplish two tasks: conversion of the data between the form used in the instrument and the parallel digital form, and management of the appropriate transfer of the parallel digital data to or from the CPU data bus. As illustrated in Fig. 2, the bus transfer process is performed by input ports and output ports [or combination input-output (I-O) ports]. Data storage in the port allows it to exchange data with the instrument in real-world time and with the computer on command from the CPU. Conversion of the data to or from parallel digital encoding requires a change in the encoding quantity or "domain" of the data.

Fortunately, there is only a limited number of ways in which data can be electrically encoded, and these fall into three categories of domains: analog, time and digital (3). Digital domain encoding has been described above. In the analog domains, the data are encoded as the magnitude of an electrical quantity (voltage, current, charge, or power). When the signal information is in the time of the signal variation rather than its amplitude, the data are in one of the time domains; data encoded as frequency or pulse width are examples. Since there are so few electrical data domains, only a few types of domain converters are needed to interface a large variety of instrument functions. As discussed below, progress in both I-O ports and conversion devices has greatly influenced the pace and nature of the development of computer-based instruments.

Attachment. In the first applications of computers to scientific instrumentation, independent and separately viable instruments and computers were simply attached together. The combination was conceptually simple, but in practice the interface for each interaction between instrument and computer was often specialized, complex, and expensive. Much of the I-O port and conversion circuitry had to be custom designed with hundreds of small components. In this stage, the computer-instrument interaction was often limited to collecting the data and controlling only the variable normally scanned by the instrument. This characterizes the attachment phase in the instrument-computer relationship. From these early associations, the power of the computer to *control* instruments as well as process data began to be appreciated.

Absorption. In recent years the task of interfacing has been greatly simplified by the availability of integrated circuit I-O ports, which permit easy connection to the CPU bus and dramatic improvements in the capability, economy, and ease of application of data conversion devices. The digital output of an analog-to-digital converter (ADC) or counter or the digital input of a digital-to-analog converter (DAC) can be connected to a parallel I-O port for a complete interface. The need for conversion devices has motivated great improvements in the cost, performance, and size factors in ADC's and DAC's for analog conversions and in digital counters and clocks for frequency and time-interval conversions. With bus support for an almost unlimited number of I-O ports and the

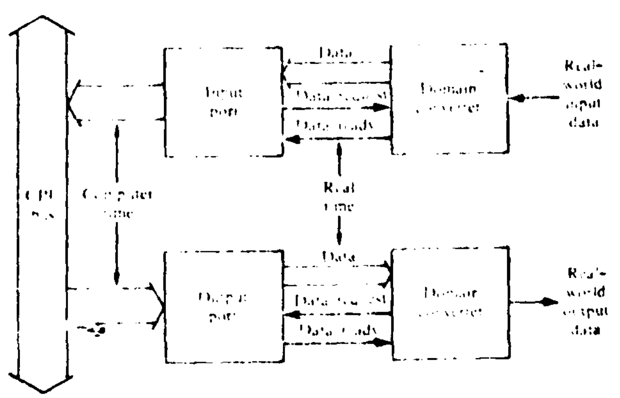


Fig. 2. Parallel I/O interface between the CPU bus and domain converters. The input and output ports connect domain converters appropriate for the real-world devices to the CPU bus. Data transfers are synchronized by the "handshaking" signals, *Data ready* and *Data request*. [From (2).]

availability of simple and inexpensive interfaces, it is easy to connect most or even all of the sensing and control elements of the instrument to the computer. This allows the computer to be involved in many more instrument functions than scanning and data collecting. For example, the computer can provide automatic selection of the measurement sensitivity for improved dynamic range and pressures and temperatures can be monitored for safe start-up, orderly shutdown, and appropriate operating conditions. If instrument controls are interfaced as well, the computer can test and adjust any or all of the instrument parameters and perform the controller function in the dynamic feedback control of these parameters (2). As more functions of the instrument are brought under computer control and the number of interfaces grows, the computer increasingly becomes an integral part of the instrument. As the distinction between computer and instrument disappears and the instrument can no longer function as an independent unit, the traditional concept of separate instrument, computer, and interface becomes obsolete. Most current examples of computers in scientific instrumentation are in this absorption phase in the instrument-computer relationship.

Transformation. Signs of the transformation stage in the relationship are emerging, however. In this phase, "computerization" of traditional instrumentation will yield to the development of new types of instruments based on principles of measurement and control that would not have been practical or possible without the integral involvement of the dedicated computer. Current examples of such instruments are three-dimensional tomography instruments and x-ray diffractometers, the Fourier transform versions of nuclear magnetic resonance (NMR), infrared, and mass spectrometers, and the combination of capillary gas chromatography and mass spectrometry. Further examples and possible future directions for the transformation stage will be explored in later sections of this article.

Turning Knobs into Keyboards

The functions and parameters of a traditional instrument are controlled by the operator through a variety of knobs, switches, levers, and valves. From these same controls and from meter displays the operator obtains information about the operating mode and performance of the instrument. This familiar mode of interaction with the instrument changes drastically when these selections, adjustments, and quantities are brought under the control or monitoring of the computer. Only for a brief time during the attachment phase were instruments made that provided a manual override for every computerized function. Dual modes of control eliminate the economic advantages of replacing mechanical controls with electrical signals. Thus to select or observe parameters that the computer controls and monitors, the operator must interact with the computer. Many devices and techniques are being used for this interaction and still more are under development, but no single "best" approach has yet been found. In this section, some of the problems and options in the interaction between operators and computerized instruments are explored.

Operator-instrument interaction. The statement that a particular function is under computer control means two things: the function is interfaced to the computer bus and there exists a set of instructions (a program) for the computer to follow to achieve the desired operation. In selecting one of the available functions of an instrument, the operator directs the computer to the program that, when executed, will implement that function. By selecting particular programs in an optical instrument, for example, the operator may select the light path configuration, the wavelength control mode (fixed, scanning, stepped), and the format in which the data will be recorded or displayed. However, before a wavelength scanning program can be run, the operator usually provides the desired wavelength range and scan rate; it is the job of yet another computer program to collect from the operator those parameters needed for execution of the selected function. The complete collection of programs for an instrument can be very complex, given the need to select modes of operation and parameter values and then to control one or more quantities while acquiring, processing, and displaying data. There are many potential computer systems that will create, edit, store, select from, retrieve, and execute the programs through which the instrument operates. The most common choices tend to follow one or the other of two models described below: that of the general-purpose computer and that of the smart process controller (4). Which of these models is used in the instrument design has a profound influence on the nature of the operator-instrument interaction.

Mini/Microcomputers. A general-purpose computer system provides ways to store a large number of programs, to modify programs; and to add new programs to the repertoire. The most common storage system is removable magnetic disk or tape because it provides a huge off-line storage capacity as well as the medium for the introduction of new programs. The desired programs, or large fragments of them, are loaded from magnetic storage into computer read-write memory prior to execution. An important part of a general-purpose computer is the operating system, a collection of programs that performs the chores of locating and transferring programs and data between memory and the magnetic storage devices. Most operating systems also include programs for editing and compiling new programs for tending common computer peripherals such as terminals, printers, and communication couplers. The operating system's programs for disk and tape management and peripheral control can also be used by the programs that control instrument operation. To support the operating system, the computer must have magnetic storage, a large amount of read-write memory, and a standard computer terminal (as in Fig. 1). Independent of the instrument, it can function as a general-purpose laboratory computer. The instrument operator then uses the computer's operating system program to call up the desired instrument programs and execute them. While this approach provides great adaptability and uses many standard computer and program modules, it requires that the instrument operator become a reasonably efficient computer operator as well.

Process controllers. A smart controller, on the other hand, need not look like a computer at all. It can take various other forms such as a calculator, a microwave oven timer, or an electronic arcade game. In a smart controller, the microprocessor part of a microcomputer (the CPU, at least) is interfaced through its bus to the instrument in the usual way. The programs needed for the desired instrument functions are contained in the processor's read-only memory

(ROM). This eliminates the need for a magnetic storage system for programs and the operating system to manage it. It also eliminates the general-purpose computer's ability to support the revision of old programs or the compilation of new ones. Some smart controllers have interchangeable ROM modules by which the manufacturer can provide new or revised functions. The keypad control panel and display can provide simple function selection by being directly labeled for the commands and messages appropriate for the options available among the instrument functions. The keypad buttons replace similarly labeled dials and switches on the traditional instrument. Most scientific instruments designed in the last few years include a microprocessor operating as a smart controller. They provide significant economies in design and manufacture and can provide substantial performance advantages in application (5).

Each of these two approaches to computerized instruments has its advantages and disadvantages. The full computer with an operating system is powerful, versatile, expandable, and also relatively expensive and usually more demanding of the operator. Impatient with the sometimes tedious process of getting to the program to change a particular parameter, some operators pine for the day when they could just reach up and twist a knob. By contrast, the smart controller is inexpensive, simpler to operate, and inherently limited in function and expandability. Knowledgeable operators are sometimes frustrated with smart controller instruments because they cannot modify an operation or check a suspected problem in the data processing program. If an instrument, such as gas chromatograph–mass spectrometer (GC-MS), produces a large quantity of data, it will require a data storage capability for which a magnetic disk is currently the best solution. In such a case, disk management software is required and the full computer with operating system is generally used to provide it. As more experience is gained and programs improve, the complexity of the operating system can be masked from the operator by a program that provides a simple set of options to the operator (like the smart controller panel) and translates the operator's actions into appropriate commands to the operating system. At the same time, smart controller instruments could be much more adaptable if new ROM modules could be programmed by the user with his laboratory computer.

Intelligence and Speed

The principal power of the computer comes, of course, from the ability of the CPU to follow a programmed sequence of simple operations at great speed. Operations that appear to be intelligent, as opposed to just fast, result from the ability of the processor to branch to different sections of the program depending on the results of its previous operations. In instrumentation applications, then, measurement or control procedures can be altered depending on the outcome of tests or measurements. The intelligence of the programmer in choosing the actions that should follow given conditions is then implemented in a dynamic way during the functioning of the instrument. The ability of the processor to test and branch (observe and respond) on the microsecond time scale allows computer-based instruments to implement "human intelligence" in operations and processes at speeds that are far beyond human capability. The following are examples of intelligent capabilities that might be found in appropriately programmed instruments:

1) Will not execute an inappropriate command.

2) Responds to high-level commands.

3) Aids operator in effective instrument use.

4) Aids operator in interpreting data.

5) Calibrates itself automatically.

6) Tests its own operation and diagnoses failure.

7) Dynamically optimizes data collection.

In each case, rather than blindly following a predetermined sequence, the computer makes decisions or interpretations which make the instrument appear to have some intelligence. For example, in a photon or particle counter, a strategy can be implemented which adjusts the times for signal and background counting to maintain constant accuracy and reduces the overall experiment time by a factor of 20 (6). Since an instrument's degree of intelligence (after it is completely interfaced) depends so much on the program sophistication, more and more of these intelligent functions are appearing in computer-based instruments. There are programs that help the operator select and load the appropriate data disk and programs that match spectra or retention times with library data, label the data display, and write a report. Self-calibration and self-diagnosis can greatly enhance reliability and reduce the required skill level of the operator.

The results produced by intelligent instruments, however, still depend on the quality and quantity of data collected. Advances in the analytical power of instrumentation can proceed along two tracks. One is that of the chemometrician who wants to make sure that all of the real information is extracted from data. The other is that of the instrumentalist who explores the possibilities of designing instruments that can provide more useful data. Both approaches are valuable and both depend, in their way, on the increased involvement of the computer.

Measurements in *N* Dimensions

A major aspect of the transformation stage is that the computer is freeing us of the limited number of variables that can be accommodated by traditional instruments. In a single-display instrument such as a *p*H meter or photometer, all system parameters are fixed except the one quantity being measured. It is assumed that the signal from the sensor is interpretable to give the sought-for quantity and is influenced by no other factors. However, there are always other factors that affect the detector output. Some affect the detector directly (as temperature and humidity can affect the characteristics of a strain gauge) and some affect the measured system so as to change the signal interpretation factors (as solution temperature affects conductivity and *p*H measurements).

Computer-enhanced detection. When only simple electronics and linear displays were available, it was necessary to choose sensors with a linear response and a minimal sensitivity to uncontrolled variables. The application of the computer to the processing of sensor signals opens many more options for measurement systems. The sensor output need no longer be linear in the measured quantity; as long as the sensor output is consistent and single-valued, the computer can interpret the data through a formula or look-up table. It is also unnecessary for the sensor output signal to stand out clearly from the background noise. The computer can average out random noise or perform other correlation functions on the signal to distinguish the noise at the sensor from the desired response. In some forms of NMR, it is routine to average thousands of sample responses to produce a spectrum that would have been buried deeply in the noise of a single response. Another point is that the computer can readily incorpo-

rate variables other than the main sensor output into the interpretation process. For example, the presence of potassium ion interferes with a sodium-specific ion electrode; an electrode specific to potassium can be added to the system and the outputs of both electrodes interpreted to give the concentrations of both ions. Further complicating the problem, the mutual interference coefficients are not exactly predictable, but even these can be determined by a standard addition and taken into account in the calculation (7). In a simpler and recently commercialized example, the temperature effect on the response factor in pH measurements has been automated by a sensing system that combines a temperature sensor with the glass electrode.

Multidimensional instruments. The application of the chart recorder to scientific instruments brought about a significant revolution in instrument design and capabilities because it added the capability of a second dimension in measurements without the necessity of recording the data on photographic films. The information output of our instruments increased dramatically (just as a spectrum contains much more information than a single absorbance measurement). Instruments that could not have existed in one dimension became a possibility (for example, the gas chromatograph). In an analogy with "Flatland" (8), the computer frees us from two dimensions, launching us into computer-aided multidimensional scientific perception. Some of the most spectacular advances in scientific instrumentation in recent years have been in multidimensional instruments.

One of the difficulties faced by the creatures of Flatland is that, viewed edge-on, the other beings; which are all regular polygons, look very much alike. They made a science of the techniques for distinguishing the shapes of others—a study in subtle clues that required years to master. These same polygons viewed from a third dimension above the plane of Flatland were, of course, easily characterized on sight. It is much the same with multidimensional instruments—what were subtle differences in two dimensions may stand out in clear distinction in three. A vivid example is computer-aided tomography (CAT), which resolves the response to a stimulus into its three-dimensional spatial coordinates. After the stimulus is scanned through one or more coordinates, a complete three-dimensional model of the response is calculated and presented. The impact of CAT on diagnostic medicine is already dramatic.

The additional dimensions do not have to be spatial, however, to be useful for improved characterization. Any sensor that detects a different characteristic of the sample or subject can provide a useful dimension. The immense success of GC-MS is due to the combination of the high resolving power of GC retention time with the highly distinctive characteristic of the mass spectrum. With an associated computer, a GC-MS instrument records mass spectra at regular increments of elution time throughout the GC run. The complete experimental data are then sometimes plotted to show their three dimensions—mass and time along the two axes in the horizontal plane and ion intensity as a contour above that plane. Clearly, the three-dimensional contour contains very much more information about the sample than exists in either the chromatogram or the mass spectrum. One of the principal advantages of the greater power of sample characterization is that the greater selectivity allows analyses to be performed with much less effort spent in sample preparation.

A number of other multidimensional instruments have also been developed recently. One example involves excitation-emission fluorescence. Figure 3 is a data plot obtained by Hershberger *et al.* (9) from an instrument that produces an emission spectrum for a whole range of excitation wavelengths. This results in the three-dimensional plot shown. This is actually for a particular time in a chromatographic elution. Thus this instrument is capable of filling a four-dimensional data matrix.

A three-dimensional instrument in which two dimensions are mass is the recently developed triple quadrupole mass spectrometer shown in Fig. 4 (10). In this instrument, ions from the source are mass-selected by the first quadrupole mass filter and then undergo an ion-molecule reaction with neutral molecules

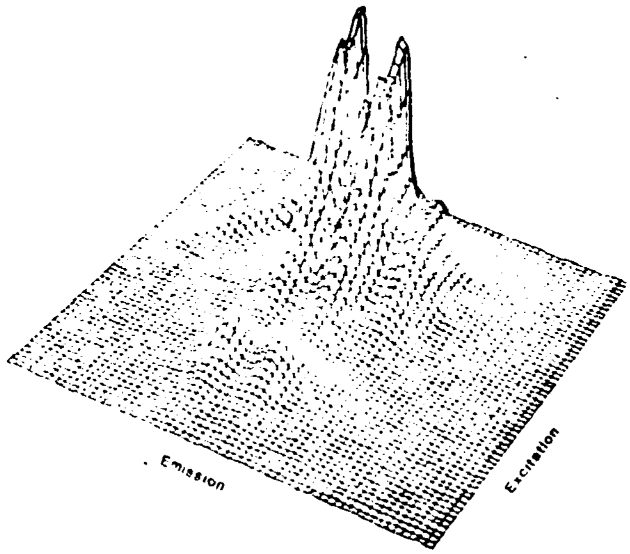


Fig. 3. Three-dimensional projection of an emission-excitation matrix corresponding to the chromatographic peak of benzo[a]pyrene from a sample of shale oil. [From (9).]

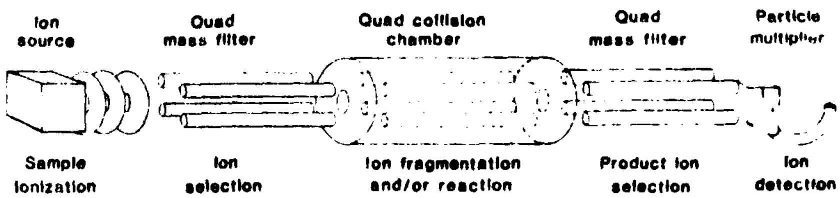


Fig. 4. Schematic of the triple quadrupole mass spectrometer (TQMS). Ions from the source that are mass-selected by the first quadrupole mass filter undergo fragmentation by collision with neutral molecules in the quadrupole collision chamber. The mass spectrum of the ionic reaction products is obtained by scanning the third quadrupole. [From (10).]

in the center quadrupole collision chamber. The center quadrupole contains the ionic reaction products but is not mass-selective. Scanning quadrupole three produces the mass spectrum of the ionic reaction products. The resulting three-dimensional information array is shown in Fig. 5 (11). The information in the ordinary mass spectrum of this compound, isopropanol, is only the peaks along the diagonal line in the foreground. The parent ion mass (selected by quadrupole one), reaction product or daughter ion mass (selected by quadrupole three), and ion intensity are the principal three dimensions. Additional dimensions of information we have found useful are the electron energy in the ion source, the kinetic energy of the parent ion, and the collision gas pressure. There are also possibilities for preselection by chromatography or selective volatilization, and selective chemistry in the ionization source and collision chamber. The total amount of information available from a single sample is thus enormous.

It is not obvious at first that the greater resolving power afforded by adding dimensions to a technique can actually increase the sensitivity of that technique. This is because, for most techniques, the sensitivity (minimum detectable quantity or property) is limited not by the ability to detect smaller amounts, but rather by the presence of other components in the system under study that affect the instrument's response. The ability to spread interfering components out in another dimension then allows the detector's inherent sensitivity to be used for the component or components of interest. For example, in the triple quadrupole mass spectrometer, the first and third quadrupoles can be set to monitor a parent-daughter mass combination that is highly characteristic of a specific sample molecule. This can provide a very sensitive detector for such an individual component in a complex mixture.

Data Collection, Data Analysis, and Intelligent Control

The great power of multidimensional instruments is also their limitation—that is, they can produce an immense amount of data about a single sample. This poses two kinds of problems: it can take a long time to collect the data, and it can take a large computer a long time to analyze them. The total number of data points in the complete data matrix increases by orders of magnitude for each added dimension. The computer in the instrument is essential to patiently perform the scanning of the several variables with reasonable efficiency. In some cases, the same computer can analyze the data, but for very large data bases, large memory and disks are required. This can be very expensive, but the alternative of shipping the data matrix to a large batch computer removes the operator from real-time interaction with the data processing. In any case, when the full multidimensional capability is used, the instrument investment per number of analyses performed is very large. This certainly restricts the applicability of multidimensional instruments for routine sample analysis, at least for now.

An alternative approach, which may follow after sufficient experience with multidimensional instruments, is to develop intelligent control software for the instrument which would help it be selective about the data that it collects. The instrument could treat the N-dimensional data matrix as potential data but only pursue those parts of it that are relevant to the desired measurement goal. The operator would specify in advance the particular characteristics of the sample that were being sought or studied by the measurement. This model is based on the fact that one usually does not want to know everything about a sample. The fraction of the total possible data that contributes to the result of interest is often very small; for instance, studies have demonstrated that only a very small fraction of the data in a mass spectrum or an infrared spectrum is needed for positive identification of a pure compound (12). Ideally, then, the analysis time could be reduced by a very large factor over the total matrix approach.

A procedure that would seek out the most relevant data might begin by performing some tests for the classes of compounds or phenomena of interest. Only the positive results would be followed up with increasingly selective

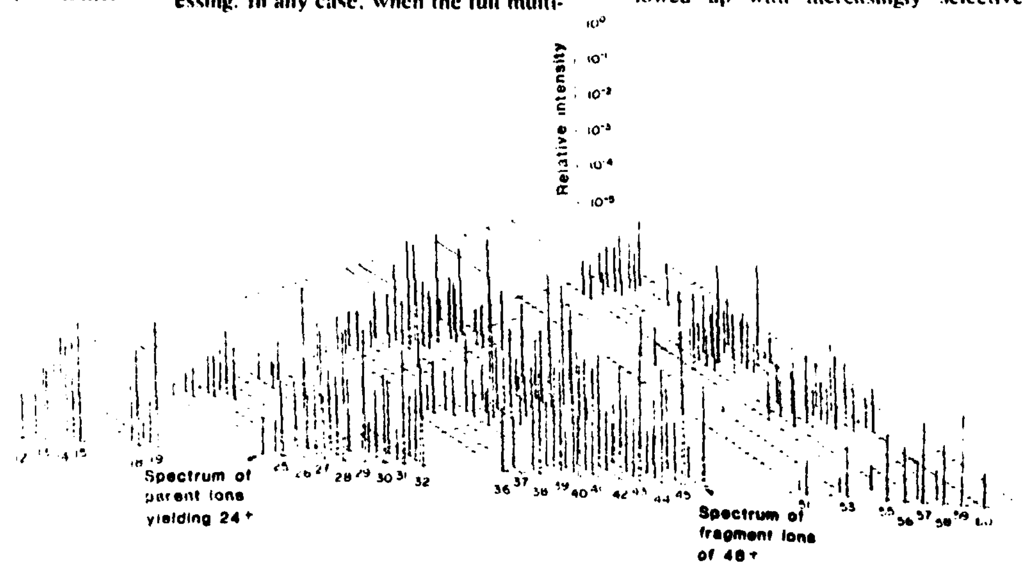


Fig. 5. Three-dimensional projection of the ions observed for all combinations of masses selected by the first and third quadrupoles in the TQMS for a sample of pure isopropanol. Different slices through this data matrix provide different kinds of information about the sample. [From (11).]

tests that terminate as soon as positive identification or accurate quantification is made. If the original goal statement leads to unsatisfying results, it must be modified and the experiment repeated. This approach would use the real-time decision-making capability of the computer to the fullest in order to keep high throughput without sacrificing the selectivity available in multidimensional instruments. It requires that the instrument parameters are tractable to computer control and that the interpretation times of the test results are short. I am not aware of any instruments that follow such a procedure at this time, but I believe they will be developed. Part of this conviction is based on the fact that it is the computer implementation of the procedure scientists follow when faced with a complex problem to solve (*13*). The "try every combination" approach is only taken when analytical reason has failed.

Distributed Intelligence and Multiprocessor Systems

It was a major step when the computer entered the laboratory as opposed to the laboratory data being carried to the computer. The concept of the "central" computer has remained, however, even in the laboratory. When additional instruments were computerized, they were often just "attached" to the same minicomputer after it was upgraded to handle multiple tasks and time-shared operations. This situation was common during the attachment phase of computer applications. In the absorption phase a dedicated computer is required for each instrument, which is economically feasible with the microprocessor. In the meantime, scientists have become accustomed to the now powerful data processing, display, storage, and programming capability of the well-developed general-purpose computer. Of course, a microprocessor can also be expanded to this capability, but then it is, in cost and fact, the same as a general-purpose computer. Some of the best of both worlds can be achieved if the dedicated microprocessor is connected, along with other microprocessor-based instruments, to the time-shared computer. This larger computer can provide and share the expensive functions of printing, plotting, storage, and high-level processing while the dedicated microprocessor tends the immediate needs of its instrument. These comprise the first two levels in a hierarchical system of distributed processing.

Communication standards. Microprocessors are now frequently used as process controllers in "smart" devices that are intended to be connected to general-purpose computers. These are subsystems of varying intelligence for which the microprocessor was a convenient building block. Examples of intelligent subsystems include many computer peripherals, graphics displays, data loggers, and a variety of electronic test instruments. Scientific instrument manufacturers are also beginning to think of instruments as elements in an extended information system rather than stand-alone devices (*14, 15*).

The development of standards for data communication among devices is greatly aiding this process. Two of these standards are now dominant: the serial asynchronous communication link with ASCII-formatted data and the IEEE-488 standard bus for programmable instrumentation (*16*). The former is the "teletype" standard for common computer peripherals, and the latter is a general purpose interface bus (GPIB), first designed by Hewlett-Packard to bring various combinations of generating and measuring instruments under common intelligent control. Instrument and computer manufacturers now provide a "488" bus connection option for almost 2000 products, which makes it relatively easy to assemble custom intelligent systems from off-the-shelf components (*17*). Properly implemented, distributed intelligence has the great advantage of allowing each processing task to be performed by the most effective processor for that task.

Parallel processing. As more complex instruments are developed, the number of high-speed and often simultaneous tasks that need to be be performed can easily exceed the capabilities of a microcomputer, or even a fairly sophisticated minicomputer. It is not necessary to run all the tasks through a single processor, especially since the CPU is one of the least expensive parts of the computer. Multiple processor systems provide increased computing power through simultaneous task execution and simplification of the task-assignment software. Distributed intelligence systems are, of course, multiple processor systems, but they are generally too loosely bound together to provide the concerted increase in computing power required by the next generation of instruments. This will probably be met by parallel processing systems—a closely linked set of processors with independent memory and functionality, but with shared communication links and peripherals. At least one supplier of modular microcomputer products (Intel) already supports a well-developed system for parallel processing. The power of parallel processing is probably essential for intelligent real-time experimental control in multidimensional instrumentation, but even without the need for parallel execution, the simplification it affords in task mixing and priority-setting may make parallel processing attractive.

The Software Problem

The cost of computing hardware has continued to plunge while computing power and ease of interfacing have increased. This has made it increasingly easy to put together the hardware to perform complex operations. However, the software required, especially for varying combinations of complex operations, is not so easily implemented. Thus as our expectations for the software have increased and hardware costs have decreased, software has rapidly become the major expense and the limiting factor in the advancement of microcomputer applications. The cost of software development is now estimated to be more than 80 percent of the total production cost of the average computer-based product (*18*). This limitation can be even more serious for scientific instrumentation, which lacks the economic base of the word processor or arcade game markets. Fundamental breakthroughs are required to solve this problem. These could come in several areas, in most of which the computer is invoked to aid in solving its own problem. One area is in the development of programs that can write programs. The description of the desired program would be given in statements more like English (*19, 20*) than like current computer languages. Another area is in the development of microcomputers that execute high-level programs directly. Such processors will speed execution, simplify programming, and further reduce hardware requirements (*21*). Still another possibility is the incorporation of more task-specific hardware such as a data logger that does not have to be programmed.

The Science of Scientific Instrumentation

I have explored in this article possible trends and capabilities for intelligent instruments in the future. If such instruments are to be available to advance science and to be applied in the social fields of energy, health, and environment, how will they be brought about? Who is going to explore these directions so that a few years from now these new capabilities will be available in our laboratories? Just as fundamental work in solid-state physics spawned the great semiconductor revolution, science often explores and explains new phenomena which the technological side of society then applies. This process is not strictly one-way, however, because it is this same technology that then supplies the tools (instruments) necessary for the next advances in science. We must recognize that the side of this cycle that reduces new science to practical devices is driven by the economy, not by scientific altruism or curiosity. That is why the sophistication in computer-based office equipment and entertainment devices is far beyond that in our latest instrumentation. It is somewhat sobering to realize that we would not have integrated circuits or microprocessors to use in our instruments at all, if it were not for the military, business, and entertainment markets. What scientists would not be excited to have the graphics capability in their instrumentation that is now commonplace in arcade games? In order to help close the loop, scientists must be involved in the feedback from technology as well as the feed forward.

Unfortunately, this has not generally been recognized as an essential function for scientists. A recent analysis, summarized in Table 1, shows that many significant scientific advances that have affected scientific instrumentation have done so 10 to 20 years after their first commercial use. Clearly, it is in the best interests of science to shorten this cycle significantly. This process could be aided greatly by ensuring that science students have the opportunity for formal education in the principles of electronics, computer science, and statistical analysis. In the subdiscipline of instrumentation, well-prepared researchers will combine solid science with the principles of electronic and computational data manipulation to develop the bases for the tools we need for the future. After all, if we are going to put intelligence in scientific instruments, it should be the scientist's intelligence we put there.

Table 1. Typical areas of technological impact (4).

Field	Theory	Inventions	Use	Instruments
Communications	1860–1900	1880–1920	1920–1940	1940–1950
Distance measure	1900	1940	1945–1955	1950–1960
Drugs	1900	1930–1940	1940–1850	1960–1970
Control systems	1930	1930–1940	1950–1970	1960–1980
Computation	1940	1940–1960	1950–1970	1970–1980

References and Notes

1. R. J. Spinrad, *Science* 158, 55 (1967).
2. H. V. Malmstadt, C. G. Enke, S. R. Crouch, *Electronics and Instrumentation for Scientists* (Benjamin/Cummings, Palo Alto, Calif., 1981).
3. C. G. Enke, *Anal. Chem.* 43, 69A (1971).
4. C. H. House, *Computer* 13, 35 (December 1980).
5. A. F. Shackil, *IEEE Spectrum* 18, 45 (April 1981).
6. E. J. Darland, G. E. Leroi, C. G. Enke, *Anal. Chem.* 52, 714 (1980).
7. C. Jochum, P. Jochum, B. R. Kowalski, *ibid.* 53, 85 (1981).
8. E. A. Abbott, *Flatland: A Romance of Many Dimensions* (ed. 2, 1884; Dover, New York, 1952).
9. L. W. Hershberger, J. B. Callis, G. D. Christian, *Anal. Chem.* 53, 971 (1981).
10. R. A. Yost and C. G. Enke, *ibid.* 51, 1251A (1979).
11. ____, *Am. Lab.* 13, 88 (June 1981).
12. R. B. Lam, S. J. Foulk, T. L. Isenhour, *Anal. Chem.* 53, 1679 (1981).
13. R. Hofstadter, *Godel, Escher, Bach: An Eternal Golden Braid* (Vintage, New York, 1979).
14. D. P. Binkley and H. W. Major, Jr., *Am. Lab.* 13, 66 (September 1981).
15. S. R. Grebel and C. E. Sharrar, *ibid.*, p. 130.
16. J. Miklosz, *Electr. Eng. Times* (26 October 1981), pp. 31–70.
17. R. E. Metzler, *Electronics* 54, 129 (11 August 1981).
18. G. Mhatre, *Electr. Eng. Times* (29 October 1979), p. 53.
19. E. Bride, *Software News* 1, 2 (5 October 1981).
20. R. C. Johnson, *Electronics* 54, 39 (7 April 1981).
21. Y. Chu and M. Abrams, *Computer* 14, 22 (July 1981).

22. This work was supported in part by the Office of Naval Research.

SP472-3/A1

472:GAN:716:ddc
78u472-608

TECHNICAL REPORT DISTRIBUTION LIST, GEN

	No. Copies
Office of Naval Research Attn: Code 472 800 North Quincy Street Arlington, Virginia 22217	2
ONR Branch Office Attn: Dr. George Sandoz 536 S. Clark Street Chicago, Illinois 60605	1
ONR Area Office Attn: Scientific Dept. 715 Broadway New York, New York 10003	1
ONR Western Regional Office 1030 East Green Street Pasadena, California 91106	1
ONR Eastern/Central Regional Office Attn: Dr. L. H. Peebles Building 114, Section D 666 Summer Street Boston, Massachusetts 02210	1
Director, Naval Research Laboratory Attn: Code 6100 Washington, D.C. 20390	1
The Assistant Secretary of the Navy (RE&S) Department of the Navy Room 4E736, Pentagon Washington, D.C. 20350	1
Commander, Naval Air Systems Command Attn: Code 310C (H. Rosenwasser) Department of the Navy Washington, D.C. 20360	1
Defense Technical Information Center Building 5, Cameron Station Alexandria, Virginia 22314	12
Dr. Fred Saalfeld Chemistry Division, Code 6100 Naval Research Laboratory Washington, D.C. 20375	1
U.S. Army Research Office Attn: CRD-AA-IP P.O. Box 1211 Research Triangle Park, N.C. 27709	1
Naval Ocean Systems Center Attn: Mr. Joe McCartney San Diego, California 92152	1
Naval Weapons Center Attn: Dr. A. B. Amster, Chemistry Division China Lake, California 93555	1
Naval Civil Engineering Laboratory Attn: Dr. R. W. Drisko Port Hueneme, California 93401	1
Department of Physics & Chemistry Naval Postgraduate School Monterey, California 93940	1
Dr. A. L. Slafkosky Scientific Advisor Commandant of the Marine Corps (Code RD-1) Washington, D.C. 20380	1
Office of Naval Research Attn: Dr. Richard S. Miller 800 N. Quincy Street Arlington, Virginia 22217	1
Naval Ship Research and Development Center Attn: Dr. G. Bosmajian, Applied Chemistry Division Annapolis, Maryland 21401	1
Naval Ocean Systems Center Attn: Dr. S. Yamamoto, Marine Sciences Division San Diego, California 91232	1
Mr. John Boyle Materials Branch Naval Ship Engineering Center Philadelphia, Pennsylvania 19112	1

TECHNICAL REPORT DISTRIBUTION LIST, GEN

	No. Copies
Dr. Rudolph J. Marcus Office of Naval Research Scientific Liaison Group American Embassy APO San Francisco 96503	1
Mr. James Kelley DTNSRDC Code 2803 Annapolis, Maryland 21402	1

TECHNICAL REPORT DISTRIBUTION LIST, 051C

	No. Copies
Dr. M. B. Denton Department of Chemistry University of Arizona Tucson, Arizona 85721	1
Dr. R. A. Osteryoung Department of Chemistry State University of New York at Buffalo Buffalo, New York 14214	1
Dr. B. R. Kowalski Department of Chemistry University of Washington Seattle, Washington 98105	1
Dr. S. P. Perone Department of Chemistry Purdue University Lafayette, Indiana 47907	1
Dr. D. L. Venezky Naval Research Laboratory Code 6130 Washington, D.C. 20375	1
Dr. H. Freiser Department of Chemistry University of Arizona Tuscon, Arizona 85721	
Dr. Fred Saalfeld Naval Research Laboratory Code 6110 Washington, D.C. 20375	1
Dr. H. Chernoff Department of Mathematics Massachusetts Institute of Technology Cambridge, Massachusetts 02139	1
Dr. K. Wilson Department of Chemistry University of California, San Diego La Jolla, California	1
Dr. A. Zirino Naval Undersea Center San Diego, California 92132	1
Dr. John Duffin United States Naval Postgraduate School Monterey, California 93940	1
Dr. G. M. Hieftje Department of Chemistry Indiana University Bloomington, Indiana 47401	1
Dr. Victor L. Rehn Naval Weapons Center Code 3813 China Lake, California 93555	1
~~Dr. Christie G. Enke~~ ~~Michigan State University~~ ~~Department of Chemistry~~ ~~East Lansing, Michigan 48824~~	1
Dr. Kent Eisentraut, MBT Air Force Materials Laboratory Wright-Patterson AFB, Ohio 45433	1
Walter G. Cox, Code 3632 Naval Underwater Systems Center Building 148 Newport, Rhode Island 02840	1
Professor Isiah M. Warner Texas A&M University Department of Chemistry College Station, Texas 77840	1
Professor George H. Morrison Cornell University Department of Chemisty Ithaca, New York 14853	1

FILMED

8